NUCLEAR DATA AND MEASUREMENTS SERIES

ANL/NDM-81

**Covariances for Neutron Cross Sections
Calculated Using a Regional Model
Based on Local-Model Fits to Experimental Data**

by

Donald L. Smith and Peter T. Guenther
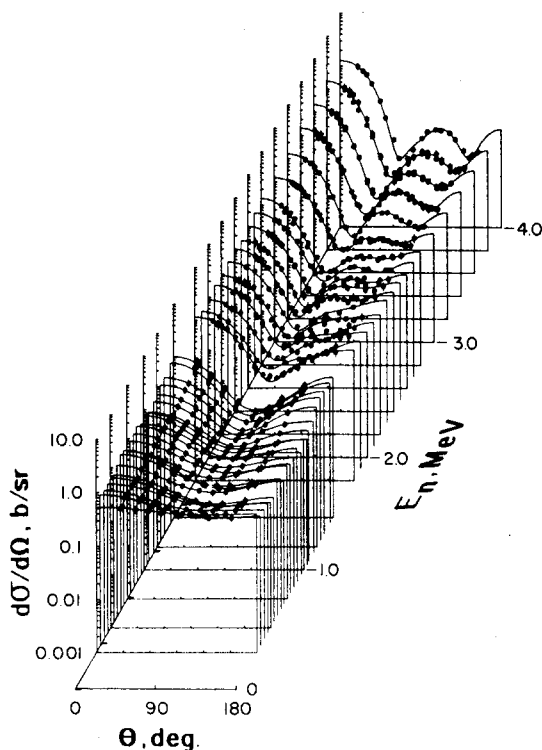
November 1983

**ARGONNE NATIONAL LABORATORY,
ARGONNE, ILLINOIS 60439, U.S.A.**

NUCLEAR DATA AND MEASUREMENTS SERIES

ANL/NDM-81

COVARIANCES FOR NEUTRON CROSS SECTIONS
CALCULATED USING A REGIONAL MODEL BASED
ON LOCAL-MODEL FITS TO EXPERIMENTAL DATA*

Donald L. Smith and Peter T. Guenther
November 1983

ARGONNE NATIONAL LABORATORY,
ARGONNE, ILLINOIS 60439, U.S.A.

The facilities of Argonne National Laboratory are owned by the United States Government. Under the terms of a contract (W-31-109-Eng-38) among the U. S. Department of Energy, Argonne Universities Association and The University of Chicago, the University employs the staff and operates the Laboratory in accordance with policies and programs formulated, approved and reviewed by the Association.

ANL/NDM-81

COVARIANCES FOR NEUTRON CROSS SECTIONS
CALCULATED USING A REGIONAL MODEL BASED
ON LOCAL-MODEL FITS TO EXPERIMENTAL DATA*

Donald L. Smith and Peter T. Guenther
November 1983

E/T

NUCLEAR MODELS. Model-parameter uncertainty esti-
mation. Covariances. Uncertainty propagation.
Experimental data fitting. Neutron cross sections.
Optical/statistical model. Code ABAREX. Z=39-51
fission product nuclei. ^{99}Tc, Ru, ^{103}Rh neutron
total cross section calculations. Experiment-model
comparisons.

Applied Physics Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439
USA

NUCLEAR DATA AND MEASUREMENTS SERIES

The Nuclear Data and Measurements Series presents results of studies in the field of microscopic nuclear data. The primary objective is the dissemination of information in the comprehensive form required for nuclear technology applications. This Series is devoted to: a) measured microscopic nuclear parameters, b) experimental techniques and facilities employed in measurements, c) the analysis, correlation and interpretation of nuclear data, and d) the evaluation of nuclear data. Contributions to this Series are reviewed to assure technical competence and, unless otherwise stated, the contents can be formally referenced. This Series does not supplant formal journal publication but it does provide the more extensive information required for technological applications (e.g., tabulated numerical data) in a timely manner.

INFORMATION ABOUT OTHER ISSUES IN THE ANL/NDM SERIES:

A list of titles and authors for reports ANL/NDM-1 through ANL/NDM-50 can be obtained by referring to any report of this series numbered ANL/NDM-51 through ANL/NDM-76. Requests for a complete list of titles or for copies of previous reports should be directed to:

Section Secretary
Applied Nuclear Physics Section
Applied Physics Division
Building 316
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439
USA

ANL/NDM-51   Measured and Evaluated Neutron Cross Sections of Elemental
Bismuth by A. Smith, P. Guenther, D. Smith and J. Whalen,
April 1980.

ANL/NDM-52   Neutron Total and Scattering Cross Sections of ^{6}Li in the Few
MeV Region by P. Guenther, A. Smith and J. Whalen, February 1980.

ANL/NDM-53   Neutron Source Investigations in Support of the Cross Section
Program at the Argonne Fast-Neutron Generator by James W. Meadows
and Donald L. Smith, May 1980.

ANL/NDM-54   The Nonelastic-Scattering Cross Sections of Elemental Nickel
by A. B. Smith, P. T. Guenther and J. F. Whalen, June 1980.

ANL/NDM-55   Thermal Neutron Calibration of a Tritium Extraction Facility
using the ^{6}Li(n,t)^{4}He/^{197}Au(n,γ)^{198}Au Cross Section Ratio for
Standardization by M. M. Bretscher and D. L. Smith, August 1980.

ANL/NDM-56   Fast-Neutron Interactions with ^{182}W, ^{184}W and ^{186}W by
P. T. Guenther, A. B. Smith and J. F. Whalen, December 1980.

ANL/NDM-57   The Total, Elastic- and Inelastic-Scattering Fast-Neutron Cross
Sections of Natural Chromium by Peter T. Guenther, Alan B. Smith
and James F. Whalen, January 1981.

ANL/NDM-58   Review of Measurement Techniques for the Neutron Capture Process
by W. P. Poenitz, August 1981.

ANL/NDM-59   Review of the Importance of the Neutron Capture Process in
Fission Reactors by Wolfgang P. Poenitz, July 1981.

ANL/NDM-60   Neutron Capture Activation Cross Sections of ^{94}Zr, ^{96}Zr, ^{98,100}Mo,
and ^{110,114,116}Cd at Thermal and 30 keV Energy by John M. Wyrick
and Wolfgang P. Poenitz, (to be published).

ANL/NDM-61 Fast-neutron Total and Scattering Cross Sections of ^{58}Ni by Carl Budtz-Jørgensen, Peter T. Guenther, Alan B. Smith and James F. Whalen, September 1981.

ANL/NDM-62 Covariance Matrices and Applications to the Field of Nuclear Data by Donald L. Smith, November 1981.

ANL/NDM-63 On Neutron Inelastic-Scattering Cross Sections of ^{232}Th, ^{233}U, ^{235}U, ^{238}U, ^{239}U, and ^{239}Pu and ^{240}Pu by Alan B. Smith and Peter T. Guenther, January 1982.

ANL/NDM-64 The Fission-Fragment Angular Distributions and Total Kinetic Energies for ^{235}U(n,f) from 0.18 to 8.83 MeV by James W. Meadows and Carl Budtz-Jørgensen, January 1982.

ANL/NDM-65 Note on the Elastic Scattering of Several-MeV Neutrons from Elemental Calcium by Alan B. Smith and Peter T. Guenther, March 1982.

ANL/NDM-66 Fast-neutron Scattering Cross Sections of Elemental Silver by Alan B. Smith and Peter T. Guenther, May 1982.

ANL/NDM-67 Non-evaluation Applications for Covariance Matrices by Donald L. Smith, July 1982.

ANL/NDM-68 Fast-neutron Total and Scattering Cross Sections of ^{103}Rh by Alan B. Smith, Peter T. Guenther and James F. Whalen, July 1982.

ANL/NDM-69 Fast-neutron Scattering Cross Sections of Elemental Zirconium by Alan B. Smith and Peter T. Guenther, December 1982.

ANL/NDM-70 Fast-neutron Total and Scattering Cross Sections of Niobium by Alan B. Smith, Peter T. Guenther and James F. Whalen, July 1982.

ANL/NDM-71 Fast-neutron Total and Scattering Cross Sections of Elemental Palladium by Alan B. Smith, Peter T. Guenther and James F. Whalen, June 1982.

ANL/NDM-72 Fast-neutron Scattering from Elemental Cadmium by Alan B. Smith and Peter T. Guenther, July 1982.

ANL/NDM-73 Fast-neutron Elastic-Scattering Cross Sections of Elemental Tin by C. Budtz-Jørgensen, Peter T. Guenther and Alan B. Smith, July 1982.

ANL/NDM-74 Evaluation of the ^{238}U Neutron Total Cross Section by Wolfgang Poenitz, Alan B. Smith and Robert Howerton, December 1982.

TABLE OF CONTENTS

PREFACE

Members of the nuclear data community are generally in agreement that uncertainty information should ultimately be provided for most evaluated nuclear data files. The methods by which this goal might be achieved are still subject to debate and are likely to require attention for some time to come.

Acceptable procedures for the evaluation of experimental data are now becoming more widely understood and implemented. Two key pragmatic considerations are: i) much of the available data from earlier work were acquired and/or documented in ways not very compatible with rigorous evaluation procedure; ii) experimenters need to be educated regarding uncertainty matters so that they will be more likely to address this aspect of their work in acceptable fashion. There remains, of course, the nagging problem of the documentation and manipulation of large quantities of uncertainty information. This is essentially a data-base-management problem rather than a physical-sciences concern.

Contemporary nuclear data evaluations rely extensively on model calculation results as well as on experimental data. Inevitably, the question of uncertainty estimation for model-calculated results must be dealt with routinely along with the corresponding issue for experimentally-derived information. The nuclear data community is aware of this matter and some attention has already been devoted to it. The present work addresses this particular problem in a modest way. The approach described here is intended to be applicable under certain circumstances, as discussed in the following text.

Uncertainty analysis is founded upon the laws of statistics and conceptually reflects our inability to acquire exact quantitative knowledge from physical observations. Observation is equivalent to experimentation, so it is not clear how one should handle the matter of uncertainty when dealing with nuclear model calculations. Uncertainty for nuclear model calculations cannot be readily compared with what we are used to considering as uncertainty for observational science. In fact, the terms "mistake" or "blunder" more readily describe the calculational experience. Computer calculational procedures are subject to limitations in precision as are experimental ones. Also, it is often necessary to explicitly introduce numerical approximation methods. These considerations can noticeably affect the outcome of nuclear cross section calculations and lead to error. However, the major source of uncertainty usually stems from the failure of models to represent physical reality, or from uncertain knowledge of the parameters for models which otherwise might be capable of doing a good job. These shortcomings and the awesome complexity typical of most nuclear model codes are serious difficulties which must be considered in developing methods for estimating uncertainties of model-calculated results.

The acquisition of a deeper understanding of physical processes and the development of correspondingly-more-sophisticated models for calculational purposes are tasks for basic research. Progress in this area will surely benefit the nuclear data field. In the meantime, the nuclear data community must work to achieve an acceptably-reliable evaluated data base for technological applications, regardless of limitations in contemporary theoretical understanding of nuclear processes.

COVARIANCES FOR NEUTRON CROSS SECTIONS
CALCULATED USING A REGIONAL MODEL BASED
ON LOCAL-MODEL FITS TO EXPERIMENTAL DATA*

by

Donald L. Smith and Peter T. Guenther

Applied Physics Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois   60439
USA

ABSTRACT

We suggest a procedure for estimating uncertainties in neutron cross
sections calculated with a nuclear model descriptive of a specific mass
region. It applies standard error propagation techniques, using a model-
parameter covariance matrix. Generally, available codes do not generate
covariance information in conjunction with their fitting algorithms. There-
fore, we resort to estimating a relative covariance matrix a posteriori
from a statistical examination of the scatter of elemental parameter values
about the regional representation. We numerically demonstrate our method by
considering an optical-statistical model analysis of a body of total and
elastic scattering data for the light fission-fragment mass region. In
this example, strong uncertainty correlations emerge and they conspire to
reduce estimated errors to some 50% of those obtained from a naive un-
correlated summation in quadrature.

I. INTRODUCTION

Models are employed extensively in nuclear science. In basic studies they provide the means for interpreting experimental results in terms of more fundamental knowledge or assumptions, and they also provide the means for predicting certain features of the outcome of experiments which have not yet been performed. In nuclear technology models are useful in representing large bodies of experimental results, and they serve to provide estimates of physical quantities which for one reason or another are impractical to measure.

The word "model" is used somewhat loosely in the literature. It therefore seems prudent to straight away make clear some nuances of its usage and substitute alternative terms to minimize possible misunderstanding of what we wish to say in this report. Perhaps in the most fundamental sense "model" implies a set of assumptions (often expressed in terms of phenomenological formulas or algorithms) which will summarize the systematics of our contemporary knowlege of certain aspects of nuclear behavior. Specific examples are the optical model (OM), the statistical model, and so forth. One might include in this category more limited schemes such as assumed nuclear level density formulas. We only rarely need to use the word in this sense and shall substitute the term "concept" in its stead.

Another use of the word "model" is in the context of model calculations. Here it implies a collection of what we have defined above as concepts. For example, the model structure (or model for short) underlying the nuclear model code ABAREX (Sections I and III) involves not only the OM concept, but also the statistical-model formulas (including level-width fluctuations), level density formulas and more. The unqualified use of "model" in the present paper alludes to this meaning. Finally one occasionally finds the term "model" used to mean the specific parameters which, when introduced into a model calculation, e.g., effectively summarize a given data base. Here we prefer the term "parameterization". It is identified as "local" if it describes an individual nucleus or element, or "regional" if is describes a number of nuclei covering a substantial mass range. An obvious difference between a local and a regional parameter is that the former has been adjusted to quantitatively describe the behavior of a specific nucleus, while the latter might be a compromise to accommodate a number of nuclei. As it turns out, a fixed constant will seldom be adequate and a parameter must be assigned a simple empirical functional form dependent upon one or more variables characteristic of the mass region investigated. A well-known example of such a "parametric enhancement" is the isospin dependence of the OM real potential. One of the key issues of this work is the relationship between local and regional parameter sets. A great deal more will be said about this later on.

Interest in the role of models in predicting quantities which are very difficult to measure is keen in the field of nuclear data because of the applied need to generate extensive evaluated results for fission and fusion reactor development purposes (e.g., Ref. 1). The role of uncertainties in experimental measurements, and in the evaluation of experimental data for applications, has been recognized and investigated extensively (e.g., Ref. 2). It is also recognized that there is a need to quantify the uncertainties associated with model calculations which are used to interpolate and/or

extrapolate the nuclear data base into regions either devoid of or sparsely represented by experimental results. The topic of model-calculation uncertainties was discussed at a 1982 workshop on covariance methods (Ref. 3). There, M. Bhat provided a useful bibliography of relevant papers; that list is reproduced in the present reference list (Refs. 4-15).

Models used in practical applications involve adjustable parameters. Physical considerations are used to limit the number and range of these parameters, and to define model structures in such a way that they represent a reasonable facsimile of what is understood about the nuclear problem at hand. In the absence of a precise understanding of nuclear dynamics, many of the models incorporate phenomenological features which have been found to be useful. From a model viewpoint, there are two distinct origins of uncertainty. One involves the uncertainty in establishing the parameterization. The other stems from an inherent failure of the model structure to represent the actual physical problem. The latter is difficult to avoid because one cannot ignore limitations resulting from fundamental ignorance. In principle, therefore, nuclear data practitioners who utilize nuclear models to interpolate (or even extrapolate) far into regions untested by observation (i.e., experimental results) should anticipate large uncertainties for their results. Furthermore, the uncertainties are hard to estimate under these conditions. On the other hand, if a parameterized model which has been adjusted to agree with experimental observations is used for predictions in circumstances not deviating excessively from the experimentally-tested domain, then the uncertainties in these predictions can be estimated with greater reliability. The situation is analogous to simple curve-fitting (e.g., Refs. 16 and 17), where intrinsic defects in the functional form of the fitted curve are compensated by parameter adjustment to match experimental reality.

Methods for fitting parameterized formulas to experimental data are discussed extensively in Refs. 16 and 17. In principle, there should be no difficulty in applying these methods to the more complex (but conceptually similar) problem of fitting experimental nuclear data with a parameterized nuclear model. For example, the OM code ABAREX by Moldauer (Ref. 18) permits the simultaneous fitting of a spherical OM to neutron total and differential scattering (elastic and/or inelastic) cross section data over a wide energy range. In practice it is rarely possible to do this rigorously. First, proper least-squares fitting analyses requires that complete covariance information be available for the input data. One seldom has this information available. Next, a rather general least-squares algorithm must be used in the fitting process. Few, if any, contemporary nuclear model codes utilize minimization algorithms designed to treat the covariances properly. Much simpler weighting techniques are normally used and correlation effects are usually ignored. Most nuclear model codes are very complex and it is impractical for all but a few who are familiar with them to modify their existing fitting algorithms. Finally, there is the matter of computational expense. Existing codes have been designed to run as quickly as possible, but even so it can become quite expensive to fit large bodies of data-especially with coupled-channel codes. Consideration of covariance information would be likely to limit further the contemporary use of these codes. In view of these very real pragmatic considerations, it becomes necessary to seek alternative (and perhaps not quite so

rigorous) schemes for fitting models and estimating uncertainties, deferring sophisticated analytical approaches until the advent of substantial progress in computer software and hardware.

Most nuclear model codes are intended to fit data for a particular nucleus, or perhaps for a multi-isotope element if one assumes an average mass A and neutron number N as an approximation. The goal for most nuclear modeling efforts in the applied nuclear data field is to develop regional parameterizations which can be used for interpolation or extrapolation to unmeasured quantities. Nuclear models involve manipulation of only a few parameters (e.g., six or fewer parameters are adjusted in most OM analyses). For the OM, it has been observed that nucleon interactions for wider ranges of nuclei can be rather well described if the parameters are assumed to be dependent on mass number A, on the neutron excess factor (N − Z), and on energy, e.g., refer to Hodgson (Ref. 19), Rapaport (Ref. 20) and Smith et al. (Refs. 21 and 22). In the absence of a fundamental understanding, simple empirical formulas are inferred from the variation in the parameters, as suggested by comparison of calculated and experimental results.

In the present work, we investigate the possibility of estimating uncertainties in regional-nuclear-model predictions based upon the actual scatter of local fitted-parameter sets relative to the regionally-predicted parameter values. It is assumed that each local parameter set serves to represent the whole body of experimental data used in the fitting process which generated that local parameter set. No a priori assumptions are made regarding specific uncertainties and correlations for these local parameters. In fact, the probable uncertainties and correlations (variances and covariances) are deduced a posteriori from consideration of the above-mentioned scatter of local parameters relative to regional predictions. It is assumed that the scatter of the local parameters relative to the corresponding regional parameters reflects all uncertainties of the procedure, including errors in the data, non-optimal local parameterization, nuclear model shortcomings, and inadequacies of the assumed model-parameter variations across the region. This line of reasoning ultimately leads to the estimation of a relative covariance matrix for the regional parameters. In turn, one can derive uncertainty estimates for cross sections, (calculated using these regional-model parameters) with the aid of standard error propagation techniques. While this approach seems quite plausible, the assumptions upon which it is based are numerous and not easily justified.

Pearlstein (Ref. 7) has also suggested a method for estimating uncertainties in fitted parameterizations. In his method, a nonlinear expression for χ^2 (which is to be minimized) is first linearized. Needed partial derivatives are derived using the model code, by means of the finite difference method. Then, in a separate (less complicated) code, the approximate χ^2 formula is used in the minimization process. This method still requires detailed covariance information for the fitted values. The need for altering the fitting algorithum of the complex model code is, however, cleverly avoided by this approach. Mass and energy-dependence can be included in this approach by expanding the number of parameters considered.

The essential difference between the method to be described in this paper and that of Pearlstein is that the present method is capable of estimating the uncertainties of a parameterization after its derivation

whereas the latter approach generates this information during the fitting process. Our approach allows the investigator to estimate uncertainty information without repeating the fitting process, details of which may no longer be accessible.

The basic ideas of the present method are developed in Section II, and formulas required for analysis are derived there as well. An example is treated in detail in Section III. It considers the regional parameterization developed for the range Z = 39 to 51 by Smith et al. (Ref. 21). Section IV summarizes the results of the present investigation. Throughout this report, the reader should remember that the terms "error" and "uncertainty" are used interchangably, and are to be interpreted as having the same meaning.

II. METHODOLOGY

The development of a reliable regional-model parameterization should be based on extensive experimental data for specific nuclei and/or elements representative of the region. In fact, this is a fundamental requisite of curve-fitting exercises, e.g., refer to Refs. 16 and 17. Therefore, we assume that experimental data are available for several nuclei or elements in the region of interest. Furthermore, we assume that these specific experimental data sets represent a relatively unbiased sampling in the region. That is to say, the nuclei considered should span the mass-region fairly uniformly. For this discussion we need not be specific about the nature of the model. However, it should be uniquely defined by a parameter set, designated here by a vector $\vec{p}$.

Assume that the model has m parameters $(p_1, p_2, \ldots, p_m)$ which are adjusted to fit data. We use the index i for this reference. Let n designate the number of distinct available experimental data sets, as discussed in the preceding paragraph. We use the index k for this reference. Furthermore, the data in these sets should be suitable for fixing the parameters of the model in question. For example, the parameters of a spherical OM can be fixed rather well for a nucleus by simultaneously fitting neutron total cross section data and differential elastic scattering data. We assume that each of the n local data sets has been fitted independently with the nuclear model code, such that each resultant parameter set is explicitly intended to provide a reasonable description of the corresponding local (elemental) data. As Fig. 1 indicates, this process reduces a collective body of n distinct experimental data sets to n local parameter vectors $\vec{p}_k$.

In order to identify a nucleus (or element) k in the region of interest, we define a coordinate vector $\vec{\alpha}_k$ which represents a collection of regional variables. We use the word "variable" rather than "parameter" to avoid confusion with the parameters which specifically serve in the model calculation. We can now consider the form of the region parameterization, which we take to be a collection of m functions p_{Ri}. Let p_{cik} be the value of p_{Ri} at $\vec{\alpha}_k$, i.e.

$$p_{cik} = p_{Ri}(\vec{\alpha}_k). \tag{1}$$

Thus, p_{cik} is the calculated regional equivalent of the local parameter value p_{ik}. When a local parameter p_{ik} is compared with a regionally derived parameter p_{cik}, this must always be done at the coordinates of the kth nucleus, $\vec{\alpha}_k$. In the specific example treated in Section III, we employ as regional variables the quantities A and (N-Z). Of course the motivation for establishing a regional parameterization in the first place is to be able to interpolate or extrapolate to nuclei not represented in the original sample.

The forms of the functions p_{Ri} are probably empirical. An explicit function p_{Ri} is generated by fitting the local values p_{ik} with an assumed functional shape (e.g., a polynomial). The nature of the regional parameterization developed this way is influenced not only by these functional forms, but also by the weighting scheme used in fitting them. We generally have no a priori knowledge of the uncertainties for the various p_{ik}. If, however, all the p_{ik} are derived in a uniform manner from data sets of equivalent scope and accuracy, then we should expect that the relative uncertainties in the various corresponding local parameters are comparable. Therefore we assume that the uncertainty Δp_{ik} can be expressed in the form

$$\Delta p_{ik} = \beta_i p_{ik}. \tag{2}$$

β_i is an unknown constant which applies to p_i regardless of the particular k. This assumption of constant fractional uncertainty for corresponding local parameters allows us to fit the regional model formulas to the local parameter sets without having to have an explicit knowledge of the β_i. Another possible fitting method would be to weight each corresponding p_{ik} equally. This method is difficult to defend because it tends to weight the larger values more heavily. There is no reason to expect that the precision to which any p_{ik} is known improves when that parameter value increases in magnitude. Thus, we chose to accept the assumption of constant fractional uncertainty for corresponding p_{ik} values in the present development.

In order to estimate errors in cross sections calculated using a nuclear model, it is necessary to have knowledge of the model-parameter covariance matrix $\bar{V}_p$ or, equivalently, the relative covariance matrix $\bar{M}_p$ since $(p_i p_j M_{pij})$ equals V_{pij} for all i and j from 1 to m. If we were to proceed under the assumption that a <u>fixed</u> set of regional parameters would serve our purpose, then V_p could be derived from a straightforward statistical analysis of the collection of local parameter sets represented by the p_{ik} ($i = 1$, m; $k = 1$, n). Unfortunately, constant regional parameters do not fit most data adequately. Thus we choose to represent our regional parameterization by m functions p_{Ri} which are fitted to the local parameter values p_{ik} and thereby reproduce observed variations across the region. Therefore, we accept as fact that most realistic collections of local parameter vectors p_k exhibit regional variations. In order to be able to do a statistical analysis on the p_{ik} (i fixed) we must renormalize the uncertainties Δp_{ik} to assure that they in fact are comparable. We do this by introducing the set of fractional-deviation quantities

$$F_{ik} \equiv \frac{p_{ik} - p_{cik}}{p_{cik}} \quad (i = 1, \text{ m}; \ k = 1, \text{ n}). \tag{3}$$

The F_{ik} are measures of the scatter of the p_{ik} about their regional equivalents, independent of their magnitudes. The samplings of the fractional deviations are really not likely to be explicitly unbiased; however, if the available fitted data sets are reasonably evenly distributed across the region of interest then the samplings can be treated as unbiased for all practical purposes.

Associated with these F_{ik} factors is a covariance matrix $\bar{V}_F$. So long as the various regional-parameter functions p_{Ri} fit their corresponding local parameter sets well, then $\bar{V}_F$ can be considered as a good approximation to M_p across the region, thus justifying our interest in the F_{ik}. The reader is referred to the Appendix where we examine the relationship between $\bar{V}_F$ and M_p in detail for a simple case in order to demonstrate these ideas.

As discussed in Ref. 23, estimates of the elements V_{Fij} for the matrix $\bar{V}_F$ can be derived from the formula

$$V_{Fij} \approx \frac{1}{n} \sum_{k=1}^{n} F_{ik} F_{jk} - \frac{1}{n^2} \left(\sum_{k=1}^{n} F_{ik} \right) \left(\sum_{k=1}^{n} F_{jk} \right) \quad (i, j = 1, m). \quad (4)$$

Eq. (4) will tend to converge as n increases. For the present consideration, $n \gtrsim 10$ is probably a reasonable sampling.

An interesting test of the goodness of fit of the regional-model formulas to the local-model parameter sets involves the terms in Eq. (4). In other notation (consistent with the Appendix) the elements of the matrix $\bar{V}_F$, namely V_{Fij}, can be expressed as

$$V_{Fij} \approx \langle F_i F_j \rangle - \langle F_i \rangle \langle F_j \rangle \quad (i, j = 1, m), \quad (5)$$

where $\langle \ldots \rangle$ designates averaging as shown explicitly in Eq. (4). The magnitude of the ratio of absolute values,

$$R_{Fij} = \left| \langle F_i F_j \rangle \right| / \left| \langle F_i \rangle \langle F_j \rangle \right| \quad (i, j = 1, m), \quad (6)$$

should be examined. Large values of R_{Fij} indicate no serious bias toward either positive or negative values for the F_{ik}, and thus a good fit. We have obtained $\bar{V}_F$ for the region of interest and can now use it to derive the covariance matrix $\bar{V}_p$ for any p calculated using the regional formulas. $\bar{V}_p$ is related to $\bar{V}_F$ by the expression

$$V_{pij} = p_i p_j M_{pij} \approx p_i p_j V_{Fij} \quad (i, j = 1, m). \quad (7)$$

It follows that the correlation matrix $\bar{C}_p$ is approximated by the corresponding matrix $\bar{C}_F$ according to the expression

$$C_{pij} \approx C_{Fij} = V_{Fij}/(V_{Fii} V_{Fjj})^{1/2} \quad (i, j = 1, m). \quad (8)$$

The rules for uncertainty propagation have been discussed extensively in the literature (e.g., Refs. 16 and 17). Let $\vec{\sigma}$ represent a set of cross sections σ_ℓ ($\ell = 1, q$) which are calculated using the regional parameterization. For the $\vec{p}$ appropriate to the nucleus in question we have

$$\sigma_\ell = \sigma_\ell(\vec{p}) \qquad (\ell = 1, q) \quad . \tag{9}$$

The covariance matrix $\bar{V}_\sigma$ for $\vec{\sigma}$ is calculated using the formula

$$V_{\sigma j \ell} = (\bar{S}_j \bullet \vec{E}_p)^t \bullet \bar{C}_p \bullet (\bar{S}_\ell \bullet \vec{E}_p) \quad (j, \ell = 1, q). \tag{10}$$

Here "$\bullet$" indicates matrix multiplication, and "t" indicates matrix transposition. $\bar{C}_p$ is calculated using Eq. (6), $\vec{E}_p$ is calculated using the formula

$$E_{pi} = (V_{pii})^{1/2} \approx p_i (V_{Fii})^{1/2} \qquad (i = 1, m), \tag{11}$$

and a typical sensitivity matrix $\bar{S}_\ell$ is given by the diagonal expression

$$\bar{S}_\ell = \begin{bmatrix} (\partial\sigma_\ell/\partial p_1) & & & & 0 \\ & (\partial\sigma_\ell/\partial p_2) & & & \\ & & \bullet & & \\ & & & \bullet & \\ 0 & & & & (\partial\sigma_\ell/\partial p_m) \end{bmatrix} \tag{12}$$
$$(\ell=1,q)$$

The partial derivatives indicated in Eq. (12) can be estimated readily using the finite difference method, with each p_i varied in turn while the other components of $\vec{p}$ are fixed. Thus,

$$(\partial\sigma_\ell/\partial p_i) \approx [\sigma_\ell(p_i + \Delta p_i) - \sigma_\ell(p_i - \Delta p_i)]/2\Delta p_i$$
$$(\ell = 1,q; \quad i = 1,m). \tag{13}$$

The analysis indicated by Eq. (13) is performed using the nuclear model code. Selection of appropriate Δp_i is guided by examination of the convergence of the finite difference expressions for various choices of the Δp_i.

Uncertainty information for the σ_ℓ derived using the regional model is contained in the matrix $\bar{V}_\sigma$. The specific errors $E_{\sigma\ell}$ are obtained from the formula

$$E_{\sigma\ell} = (V_{\sigma\ell\ell})^{1/2} \quad (\ell = 1,q). \tag{14}$$

The uncertainty correlation between σ_j and σ_ℓ is given by

$$C_{\sigma j \ell} = V_{\sigma j \ell}/(V_{\sigma j j} V_{\sigma \ell \ell})^{1/2}$$
$$(j,\ell = 1,q) \tag{15}$$

This error propagation process is indicated schematically in Fig. 1.

In this formalism the various samplings of parameter space, which are placed on equivalent footing by considering the F_{ik} rather than the P_{ik}, are assumed independent. This, of course, does not exclude the possibility of correlations between the one or more parameters. For example, in analyses with the spherical OM one should expect to observe the well-known correlation between V and r_v (often referred to as the Vr_v^2 effect, as in Ref. 7).

One obvious feature of the present approach is that a rather extensive experimental data base is needed. The number n of samplings should be large enough so that Eq. (4) yields a reasonable estimation of the elements of the parameter relative covariance matrix. There are extensive data available for certain types of cross sections, e.g., the neutron total cross section and elastic scattering cross section. For other data types the situation is less favorable. Another problem which can limit the applicability of the method is that it is not always possible to find sufficient data of comparable quality to provide adequate coverage of a region of interest. Such situations do not satisfy the present requirement that each experimental sampling be more or less equivalent, and they would require alteration of the formalism. A priori specification of uncertainties for various components of such data bases would be needed.

Unlike an arbitrary curve fitting procedure, the fitting of a model is inherently more stable due to the fundamental constraints stemming from the model's theoretical foundations. The utility of a good nuclear model lies in its power to predict a wide spectrum of physical quantities which may or may not have been included in the data base employed in its parameterization. Two rather distinctive aspects of the accuracy of predictions by a fitted model are of concern. These involve statistical features of the fitting process and the quality of the theoretical concepts of the model. These ideas can be illustrated by considering an optical-statistical model parameterization based on neutron elastic scattering data $(d\sigma_{el}/d\Omega)$ only. If we were then to calculate the elastic scattering from a nucleus not included in the original sampling, the reliability of this prediction would be dominated by statistical considerations, as discussed in this paper. If we now attempt to predict a neutron total cross section (σ_T), the outcome would be strongly influenced by the fidelity of the model above and beyond the statistical considerations. Clearly our present method cannot account for this type of uncertainty. It happens that the example we have presented does not strain the predictive capabilities of the model considered. Had we demanded instead that the model fit total cross section data, and then asked for elastic scattering distributions, the results would have been far less reliable. Clearly the present approach must be applied thoughtfully.

III. AN EXAMPLE

Smith et al. (Refs. 24-34) recently completed an extensive program of measuring total and scattering cross sections for elements in the range Z = 39 to 51. These results, supplemented by total cross section data from Poenitz and Whalen (Ref. 35), were used to develop a series of energy-dependent spherical OM parameterizations, one for each of the eleven elements Y, Zr, Nb, Mo, Rh, Pd, Ag, Cd, In, Sn and Sb. These parameter sets were derived using the OM program ABAREX (Ref. 18) which simultaneously fitted total and scattering data (mostly elastic), element by element. Subsequently, Smith et al. (Ref. 21, hereafter referred to as "Smith et al.") examined the systematic behavior of these elemental (local) parameter sets and developed a regional parameterization for the range Z = 39 to 51, inclusive of mass-, isotopic-and shell-dependent effects. Since this comprehensive body of results was derived without consideration of uncertainties, it offers a good opportunity to apply the present ideas to a typical situation as we envision it. The principal requirements for the present method appear to be satisfied. The sampling is of adequate size (eleven elements) and it spans the Z = 39 to 51 region rather uniformly. The available data cover the energy range from a few hundred keV to ~ 4 MeV in detail. Finally, all the measurements were performed in the same laboratory with more-or-less uniform precision.

Although the interested reader is referred to the papers of Smith et al. for details, we briefly summarize the salient features of their model fitting. Their OM potential employed the Woods-Saxon form for the real potential with a linearly energy-dependent depth, the derivative form for the imaginary potential with energy-independent depth, and distinct geometric parameters (i.e., r and a) for the real and imaginary potentials. The spin orbit potential was of the Thomas form with fixed depth and geometric parameters identical to those for the real potential. In comparing the potentials of various elements, they took the real and imaginary volume integrals per nucleon, $(J/A)_V$ and $(J/A)_W$ respectively, to be more meaningful measures of the OM strengths than the depths V and W (e.g., Refs. 20 and 21). For this purpose they used the approximations given in Ref. 7, which are accurate to better than one percent in the present context (Ref. 22).

Smith et al. utilized code ABAREX for the elemental model fitting. The code searches the parameter space $(V, r_V, a_V, W, r_W, a_W)$, weighting the scattering data by a factor of 10 more than the total cross section data. The results of this analysis are reproduced in Table 1. They were used to derive $(J/A)_V$ and $(J/A)_W$ values. This collection of local parameters served as the basis in developing a regional parameterization. The empirical formulas for all regional parameters, with the exception of W, were assumed to exhibit a simple linear dependence on the regional variables A or (N-Z)/A. The geometric parameters r_V, a_V, r_W, a_W were linear in A, while V displayed the well-known isovector component which is linear in (N-Z)/A. The elemental values were least-squares fitted with uniform weighting using these linear forms. The regional parameterization indicated in Table 2·A resulted. The regional empirical formula for W was taken as

the superposition of a linear isovector term (like that for V) and a cosine term whose argument depended linearly on A. As discussed in detail by Smith et al., the latter term is a convenient computational device for representing the observed shell closure dependence of W, but it has no apparent physical justification. In deriving the numerical values for the regional parameterization of W, Smith et al. proceeded in two steps using graphical methods. First they observed that $(J/A)_w$ displayed nodes around the shell closures N=50 and Z=50. Assuming the shell effect to be negligible at these points, they obtained the isoscalar and isovector components. Next they established the period of the cosine term by noting that the average A for the N=50 nuclei is 89.6, while that for the Z=50 nuclei is 118.8, implying a period of 29.2. The magnitude was then adjusted to a value that appeared to represent the elemental $(J/A)_w$ well to within the uncertainty of the entire procedure. Their judgment is also reflected in round-off accuracy of two digits to be found in Table 2.A. This parameterization will be referred to as Set A.

Our derivation of the regional parameterization differs from that of Smith et al. in two fundamental respects. First, we elected to deal with V and W rather than $(J/A)_v$ and $(J/A)_w$ because V and W are two potential parameters explicitly adjusted by ABAREX and therefore they stand on equal footing with the geometric parameters (labeled r and a). As it was emphasized in Section II, the uniform treatment of all parameters is essential to the validity of the present method. Secondly, all empirical regional formulas were least-squares fitted to the local parameters assuming uniform fractional uncertainties as discussed in Section II. As the point of departure for our analysis we accepted both the local parameters and the regional empirical formulations of Smith et al. We investigated the effect of using V and W rather than $(J/A)_v$ and $(J/A)w$ (as well as least-squares fitting the formula for W) by doing the fits with unit weights, as Smith et al. had done. We label these results Set B and show them in Table 2.B.

We then fitted the elemental parameter sets assuming that each corresponding value has the same fractional uncertainty, consistent with the tenets set forth in Section II. The regional model formulas appearing in Table 2.C, and designated as Set C, were thus obtained.

Our major emphasis in the present investigation is on analysis involving the Set C regional parameterization. Utilizing the Set C formulas and the elemental parameters from Table 1, we derived the matrix $\bar{V}_F$ according to Eq. (4). The result appears in Table 3. The estimated uncertainties (standard deviations) in the regional parameters given by the Set C formulation are also given. Furthermore, it is seen that there are several strong correlations (or anticorrelations for a negative sign). The most prominent involve the pairs of parameters (V_o, r_V)* and (W, a_W). These are well-known correlation effects for the OM (e.g., Refs. 7 and 21).

---

*Here we designate the energy-independent component of the real potential as V_o.

In the case of (V_0, r_V), it has been observed that the quantity $V_0 r_V^2$ behaves roughly as an invariant in OM studies. This is consistent with the 88% anticorrelation derived in the present analysis. The quality of the fit of the regional-model Set C to the elemental parameters can be measured by examining the R_{Fij}, as defined in Eq. (8). These values appear in Table 3 also, and they indicate that Set C forms a reasonable set of fitted curves.

As a first step is assessing the results of our analysis, we compared the total cross sections calculated using the local parameters given in Table 1 with the experimental data base of Smith et al. (Refs. 24-34). Table 4 shows the observed systematic differences over coarse energy intervals. While agreement is generally to within 2-4%, which is on the order of the experimental errors, there are some noticeable differences. We suspect that these originate because the total cross section was not given primary emphasis in the fitting process.

Next, we examine how the various corresponding parameters, computed from the Set A, Set B and Set C formulations, compare with each other and with the local parameters. Scale indicators for this intercomparison are the parameter standard deviations from Table 3. The results appear in Table 5. We note that the scatter of the elemental parameters relative to the Set C values appears consistent with the derived standard deviations. Several of these differences exceed the corresponding standard deviations for these parameters, as might be statistically expected. The differences between the values for Set A, Set B and Set C are all smaller than the corresponding standard deviations, usually substantially smaller. The difference between the parameters from Set A and Set B are quite small, except for a_V and W where the differences are noticeable but not unreasonable. The origin of the difference between Set A and corresponding Set B values for a_V is not clear. The same method of derivation was used in each instance. However, distinct methods were used in treating W so differences in these results were anticipated.

We also examined neutron total cross sections over the 1-4 MeV range for the eleven elements, using the local as well as all regional parameter sets. The results are presented in Table 6. Generally, the regional parameterizations produce lower total cross sections than the local ones. Mutual differences are usually < 4%.

Finally, we sought to determine which parameterization best represents experimental values. The answer is given in Table 7. While no one parameter set clearly fits the experimental data best, Set C evidently does worst.

Error prediction is the primary objective of this paper, so we pursued this task in the framework of the present example using the Set C parameterization throughout. First we tested self consistency by comparing our predicted uncertainties with the deviations of model predictions from experimental data for a member of the original eleven-element data base, namely Rhodium.

A search in CINDA (Ref. 36) revealed that the only other total cross section data available at these energies were from Poenitz and Whalen (Ref. 35) and Foster and Glasgow (Ref. 37). These experimental data are plotted in Fig. 2. Also shown are curves calculated using parameter Sets A, B, and C. The uncertainties predicted by our method are designated by heavy error bars centered about the Set C curve at the whole-MeV energies. These uncertainties are somewhat larger than 2%. An inspection of this figure indicates that the deviations of calculated values from the experimental ones are consistent with this uncertainty.

Next we tested the predictive capabilities of our method by considering two elements in the present mass range, but not included in the sample: Technitium and Ruthenium. According to CINDA (Ref. 36) the only available experimental data relevant to the present example are the total cross section values of Foster and Glosgow (Ref. 37). These data are plotted in Figs. 3 and 4, for Technitium and Ruthenium respectively, along with curves calculated using parameter Sets A, B and C. The predicted uncertainties are computed and shown here in the same manner as for Rhodium. The errors are generally ~ 2-3%, and again they are consistent with the deviations observed between calculation and experiment.

These observations are quantitatively stated in Table 8 together with the correlation matrix elements. The correlations vary from element to element, and this is caused by local variations in the computed sensitivity coefficients. However, in each instance the effect of the OM-parameter uncertainty correlations is to reduce the calculated error by approximately 50%. In the specific case of Rhodium, neglect of all OM-parameter uncertainty correlations leads to predicted errors in the range 4.5 - 7% compared to the 2.1 - 2.3% values from Table 8.

IV. SUMMARY

In principle, nuclear models could be fitted by rigorous least-squares methods to experimental data, thereby yielding unbiased best-estimate parameter sets along with the covariance information needed for subsequent determination of errors in other calculated cross sections. In practice, the absence of covariance information for the fitted data and inherent limitations of the fitting algorithms in most contemporary model codes imposes a need to resort to less rigorous schemes in order to estimate errors for calculated quantities. This report describes one such method.

Given a specific mass region, our method involves consideration of parameters derived from conventional analysis of experimental data, applied to several elements which collectively represent the region they span. Since model parameters are prone to vary in magnitude across a mass region, it becomes necessary to perform a transformation from the parameter space to another space which allows the use of simple statistical methods. The transformation is accomplished by selecting specific functions which represent the main features of the parameters across the region. Statistical analysis of the transformed quantities leads to an estimate of the model parameter covariance matrix which must be known in order to derive the errors in quantities calculated using the nuclear model.

The method provides the most reliable error estimates when one deals with those quantities akin to the experimental data base upon which the model parameterization is founded. Of course it will also provide estimates of errors for other cross sections calculable by the model, but the reliability of these estimates will be difficult to ascertain. In other words, the errors calculated here include only statistically based components of parametric origin. The utility of the specific model (as manifested by its parameterization) in any untested situation cannot be assessed quantitatively. Therefore, discretion must be employed in performing such analyses.

Our procedure has been demonstrated numerically in a realistic problem. This exercise clearly exhibits the importance of parameter uncertainty correlations. In our example, it is found that neglect of these correlations leads to overestimation of total cross section errors by about a factor of two, whereas inclusion of these correlations results in errors consistent with observed differences between experimental and calculated values.

ACKNOWLEDGMENT

APPENDIX

The idea that an a posteriori examination of the scatter of sampled values about the assumed best representation of the ensemble will lead to an estimate of the variance of the quantity can be better understood from a consideration of the following simple example.

Let $\{p_k\}$ be a set of n quantities obtained as a result of sampling the universe of all possible values for p; for simplicity assume them to all be <u>comparable</u> and assign equal weight to all the samples. Adopting the notation that a bar over a quantity denotes the true universal average of that quantity, we define the approximation

$$\bar{p} \approx \langle p \rangle \equiv \frac{1}{n} \sum_{k=1}^{n} p_k \qquad (A.1)$$

According to Ref. 23, the variance V_p of p is given by

$$V_p = \overline{p^2} - \overline{p}^2 \qquad (A.2)$$
$$\approx \langle p^2 \rangle - \langle p \rangle^2,$$

where the $\langle \cdots \rangle$ are to be interpreted as defined in Eq. (A.1). Following Ref. 16, we note the definition of the relative variance M_p, namely,

$$V_p = \overline{p}^2 \, M_p. \qquad (A.3)$$

Note that only one quantity is considered so the variance and relative variance are two scalar quantities rather then matrices.

Suppose that for some reason we had not bothered to try and seek the best value for p, namely $\bar{p}$ or its approximation $\langle p \rangle$, by rigorous means. Instead, assume that we obtained a value p_0 which in fact turns out to differ only a little from either $\bar{p}$ or $\langle p \rangle$. For example, perhaps we might have drawn a straight horizontal eyeguide line through a convenient graphical representation of the set $\{p_k\}$. This is an artificial situation since $\langle p \rangle$ is so easy to derive in this simple example that we would not be likely to settle for a less rigorous approximate value. However, in more complicated situations such as those discussed in the main text we may be forced by practical considerations to settle for another estimated "best value", like p_0.

Now, define the set $\{F_k\}$ by the equation

$$F_k = (p_k - p_0)/p_0 \qquad (k = 1,n). \qquad (A.4)$$

Given p_0, this unambiguously defines a transformation from the $\{p_k\}$ to the $\{F_k\}$. The variance of F is estimated from the sampling $\{F_k\}$ by

$$V_F = \overline{F^2} - \overline{F}^2$$

$$\approx \langle F^2 \rangle - \langle F \rangle^2, \tag{A.5}$$

analogous to Eq. (A.2). Combining Eqs. (A.2), (A.4) and (A.5) leads to

$$V_F = \overline{F^2} - \overline{F}^2$$

$$= \frac{1}{p_0{}^2} (\overline{p^2} - 2\overline{p}\,p_0 + p_0{}^2) - \frac{1}{p_0{}^2} (\overline{p} - p_0)^2 \tag{A.6}$$

$$= \frac{1}{p_0{}^2} (\overline{p^2} - \overline{p}^2)$$

$$= V_p/p_0{}^2 .$$

Comparing Eqs. (A.3) and (A.6) gives us the expression

$$p_0{}^2 V_F = \overline{p}^2 M_p, \tag{A.7}$$

which implies the important conclusion that

$$M_p \approx V_F \text{ if } p_0 \approx \overline{p}. \tag{A.8}$$

In this simple example, V_p can be estimated directly from the formula

$$V_p \approx p_0{}^2 (\langle F^2 \rangle - \langle F \rangle^2) \tag{A.9}$$

which follows from Eqs. (A.5) and (A.6). Eq. (A.9) applies regardless of whether or not p_0 is a good approximation to $\overline{p}$. This is always the case if p can be thought of as essentially a constant quantity. However, in the treatment presented in Section II of the text, we do not deal with such constant quantities. Instead, quantities like p are likely to vary considerably across the region. Then we must replace p_0 by an assumed function p_R and Eq. (A.4) assumes the form

$$F_k = [p_k - p_R(\vec{\alpha}_k)]/p_R(\vec{\alpha}_k), \qquad\qquad (A.10)$$

with $\vec{\alpha}_k$ identifying the regional location of sample k. Under these conditions, the transformation from $\{p_k\}$ to $\{F_k\}$ by means of the function p_R is necessary in order to be able to perform the statistical analysis needed to estimate the covariance V_p. A statistical analysis of F yields V_F which approximates M_p. Then V_p is obtained according to

$$\begin{aligned} V_p &= p^2\, M_p \\ &\approx p^2\, V_F \end{aligned} \qquad\qquad (A.11)$$

The quality of this estimate of V_p depends on the degree to which the function p_R represents the p_k values well.

REFERENCES

1. "Proceedings of the Conference on Nuclear Data Evaluation Methods and Procedures," eds. B. A. Magurno and S. Pearlstein, September 22-25, 1980, Brookhaven National Laboratory, BNL-NCS-51363 Vols. I and II, Brookhaven National Laboratory, Upton, New York 11973, USA.

2. R. W. Peele and T. W. Burrows, "An Annotated Bibliography Covering Generation and Use of Evaluated Cross Section Uncertainty Files," BNL-NCS-51684, Brookhaven National Laboratory, Upton, NY 11973, USA (1983).

3. "Workshop on Covariance Methods and Their Application to General Purpose Evaluations", compiled by Edward D. Arthur, Oak Ridge National Laboratory, May 17-18, 1982, Los Alamos Nuclear Data Group Informal Report T-2-IR(82)-1, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA (1982).

4. S. Tagesen, et al., "Evaluation of the Cross Sections for the Reactions ^{24}Mg (n,p) ^{24}Na-----," ISSN 0344-8401, ZAED 13-1 (1979).

5. B. Strohmaier, et al., "Evaluation of the Cross Section for the Reactions ^{19}F (n,2n)^{18}F------," ISSN 0344-8401, ZAED 13-2 (1980).

6. S. Pearlstein, "Analysis of Neutron Emission Spectra from 14-MeV Neutron Reactions," Nucl. Sci, Eng. __68__, 55 (1978).

7. S. Pearlstein, "Optical Model Parameters for Neutron Cross-Sections for Medium Mass Nuclei in the Energy Range 4-20 MeV and Iron in the Energy Range 4-100 MeV," Nucl. Sci. Eng. __83__, 312 (1983).

8. J. B. Dragt and H. Gruppelaar, "Error Analysis of Neutron Capture Group Cross Sections for Fast Reactors, Applied to Fission Products," RCN-192, EURFNR-1132 (1973).

9. H. Gruppelaar, "Error Calculation of Capture Cross Sections for Fission Product Nuclei," Proc. Symp. Neutron Capture Gamma Ray Spectroscopy, Petten, p. 760 (1974).

10. H. Gruppelaar, "Uncertainty Estimates of Statistical Theory Calculations of Neutron Capture Cross Sections of Fission Product Nuclei," Proc. IAEA Consultants Meeting on the Use of Nuclear Theory in Neutron Nuclear Data Evaluation, Trieste, IAEA-190, Vol. II, p. 61 (1975).

11. J. B. Dragt, et al., "Methods of Adjustment and Error Evaluation of Neutron Capture Cross Sections", Nucl. Sci. and Eng. __62__, 17 (1977).

12. A. D. MacKellar and R. E. Schenter, "Optical Model Studies for Fast Neutron Capture Cross Sections Calculations, "HEDL-TME 71-154 (1972).

13. F. Schmittroth, "Analysis of Errors in Computed Integral Cross Sections due to Fluctuating Resonance Parameters," HEDL-TME 72-99 (1972).

14. F. Schmittroth, "Neutron Resonance Spacings for Spherical Nuclei," HEDL-TME 73-30 (1973).

15. F. Schmittroth, "Neutron Capture Calculations for $E_n = 100$ keV to 4 MeV," HEDL-TME 73-79 (1973).

16. Donald L. Smith, "Covariance Matrices and Applications to the Field of Nuclear Data," ANL/NDM-62, Argonne National Laboratory, Argonne, Illinois 60439, USA (1981).

17. Donald L. Smith, "Nonevaluation Applications for Covariance Matrices," ANL/NDM-67, Argonne National Laboratory, Argonne, Illinois 60439, USA (1982).

18. P. A. Moldauer, Argonne National Laboratory, Argonne, Illinois 60439, USA (unpublished).

19. P. E. Hodgson, Nuclear Reactions and Nuclear Structure, Clarendon Press, Oxford (1971).

20. J. Rapaport, Physics Reports 87, 25 (1982).

21. A. B. Smith, P. T. Guenther, and J. F. Whalen, "The Optical Model of Few-MeV Neutron Elastic-Scattering from Z=39 to 51," to be published in Nuclear Physics.

22. A. B. Smith, Argonne National Laboratory, Argonne, Illinois 60439, USA (private communication).

23. D. L. Smith, "Matrix Formalism for Uncertainty Analysis," Rev. Sci. Instrum. 54, (7), 818 (1983).

24. A. B. Smith and P. T. Guenther, "Fast-Neutron Scattering Cross Sections of Elemental Silver," ANL/NDM-66, Argonne National Laboratory, Argonne, Illinois 60439, USA (1982).

25. A. B. Smith and P. T. Guenther, "Fast-Neutron Total and Scattering Cross Sections of ^{103}Rh," ANL/NDM-68, Argonne National Laboratory, Argonne, Illinois 60439, USA (1982).

26. A. B. Smith and P. T. Guenther, "Fast-Neutron Scattering Cross Sections of Elemental Zirconium," ANL/NDM-69, Argonne National Laboratory, Argonne, Illinois 60439, USA (1982).

27. A. B. Smith, P. T. Guenther, and J. F. Whalen, "Fast-Neutron Total and Scattering Cross Sections of Niobium," ANL/NDM-70, Argonne National Laboratory Argonne, Illinois, 60439, USA (1982).

28. A. B. Smith, P. T. Guenther, and J. F. Whalen, "Fast-Neutron Total and Scattering Cross Sections of Elemental Palladium," ANL/NDM-71, Argonne National Laboratory, Argonne, Illinois 60439, USA (1982).

29. A. B. Smith and P. T. Guenther, "Fast-Neutron Scattering from Elemental Cadmium," ANL/NDM-72, Argonne National Laboratory, Argonne, Illinois 60439, USA (1982).

30. C. Budtz-Jørgensen, P. Guenther, and A. B. Smith, "Fast-Neutron Elastic-Scattering Cross Sections of Elemental Tin," ANL/NDM-73, Argonne National Laboratory, Argonne, Illinois 60439, USA (1982).

31. A. B. Smith, P. T. Guenther and J. F. Whalen, "Neutron Total and Scattering Cross Sections of Elemental Antimony," ANL/NDM-75, Argonne National Laboratory, Argonne, Illinois 60439, USA (1982).

32. A. B. Smith, and P. T. Guenther, "Scattering of Fast-Neutron from Elemental Molybdenum," ANL/NDM-76, Argonne National Laboratory, Argonne, Illinois 60439, USA (1982).

33. Fast-Neutron Total and Elastic-Scattering Cross Sections of Elemental Indium," ANL/NDM-78, Argonne National Laboratory, Argonne, Illinois 60439, USA (1982).

34. C. Budtz-Jørgensen, P. Guenther, and A. B. Smith, "Few-MeV Neutrons Incident on Yttrium," ANL/NDM-79, Argonne National Laboratory, Argonne Illinois 60439, USA (1983).

35. W. P. Poenitz and J. F. Whalen, "Neutron Total Cross Section Measurements in the Energy Region from 47 keV to 20 MeV," ANL/NDM-80, Argonne National Laboratory, Argonne, Illinois 60439, USA (1983).

36. "An Index to the Literature on Microscopic Neutron Data," CINDA-A (1935-1976), CINDA-82 (1977-1982), and CINDA 82 – Supplement, International Atomic Energy Agency, Vienna, Austria.

C-3
37. D. G. Foster, Jr. and D. W. Glasgow, Physical Review 63, 576 (1971).

TABLE 1. Elemental Optical-Model Parameters[a]

Element	Z	A	$\frac{N-Z}{A}$	V_o	r_V	a_V	W	r_W	a_W
Y	39	89	0.124	49.19	1.230	0.738	8.143	1.471	0.303
Zr	40	$\overline{91.6}$[b]	0.127	49.41	1.221	0.748	7.680	1.416	0.398
Nb	41	93	0.118	49.71	1.230	0.702	6.505	1.349	0.477
Mo	42	$\overline{96.03}$[b]	0.125	49.86	1.207	0.767	8.093	1.399	0.438
Rh	45	103	0.126	46.90	1.266	0.686	10.990	1.319	0.431
Pd	46	$\overline{106.5}$[b]	0.136	47.35	1.260	0.637	10.160	1.230	0.527
Ag	47	$\overline{108}$[b]	0.130	48.25	1.249	0.603	8.501	1.270	0.575
Cd	48	$\overline{112.5}$[b]	0.147	48.82	1.247	0.600	7.373	1.193	0.595
In	49	115	0.148	47.29	1.267	0.644	8.496	1.317	0.406
Sn	50	$\overline{118.8}$[b]	0.158	48.53	1.251	0.596	7.040	1.244	0.471
Sb	51	$\overline{121.85}$[b]	0.163	48.36	1.245	0.620	5.600	1.210	0.627

[a]From the work of Smith et al. (Refs. 24-34).

[b]Average masses used when more than one isotope contributed significantly to OM analysis (Refs. 24-34).

TABLE 2. Regional Optical-Model Parameter Formulas

Set A: Smith et al.[a]

V_O = 52.58 - 30.0 (N-Z)/A
r_V = 1.131 + 0.00107A
a_V = 1.203 - 0.00511A
W = 11.70 - 25.0 (N-Z)/A - 1.8 $\cos\left[2\pi(A-90)/29\right]$
r_W = 2.028 - 0.00683A
a_W = -0.1061 + 0.005551A

Set B: Present work, equal weighting

V_O = 51.505 - 21.892 (N-Z)/A
r_V = 1.1311 + 0.0010658A
a_V = 1.1750 - 0.0048335A
W = 11.369 - 21.408 (N-Z)/A - 1.4464 $\cos\left[2\pi(A-89.6)/29.2\right]$
r_W = 2.0280 - 0.0068291A
a_W = -0.10774 + 0.0055682A

Set C: Present work, equal fractional uncertainty

V_O = 51.310 - 20.722 (N-Z)/A
r_V = 1.1296 + 0.0010767A
a_V = 1.1585 - 0.0047023A
W = 11.605 - 24.709 (N-Z)/A - 1.3921 $\cos\left[2\pi(A - 89.6)/29.2\right]$
r_W = 2.0093 - 0.0066807A
a_W = -0.12986 + 0.0055749A

[a]Ref. 21

TABLE 3. Optical-Model Relative Covariance Matrix Results.

Parameter	Error[a]	Correlation Matrix[b]					
		P_1	P_2	P_3	P_4	P_5	P_6
$P_1 = V_o$	1.9%	1			(symmetric)		
$P_2 = r_V$	1.1%	-0.88	1				
$P_3 = a_V$	4.5%	0.17	-0.41	1			
$P_4 = W$	11.5%	-0.47	0.50	0.20	1		
$P_5 = r_W$	3.4%	0.08	-0.14	0.64	0.53	1	
$P_6 = a_W$	15.0%	0.23	-0.27	-0.39	-0.89	-0.81	1

Quality of Fit Parameters[c]

i	j	R_{Fij}	i	j	R_{Fij}
1	1	687.4	3	3	125.9
1	2	1002	3	4	10.55
1	3	51.59	3	5	105.8
1	4	52.57	3	6	12.85
1	5	30.21	4	4	19.97
1	6	20.41	4	5	34.42
2	2	1888	4	6	11.24
2	3	198.2	5	5	213.5
2	4	95.20	5	6	36.30
2	5	90.07	6	6	11.03
2	6	36.34			

[a]Error in P_i is derived from $(V_{Fii})^{1/2}$, expressed in percent, using Eq. (4).

[b]The correlation matrix elements are calculated using Eq. (8).

[c]Derived using Eq. (6). $R_{Fij} = R_{Fji}$ for all i, j = 1,6.

TABLE 4.   Comparison of Total Cross Section Experimental Data and the
Predictions of the Fitted Elemental Model Formulations.

Element	Trend of Experimental Data Relative to OM Results[a]			Maximum Difference[b]
	1 – 2 MeV	2 – 3 MeV	3 – 4 MeV	
Yttrium	+	0(+)	+	+ 6%
Zirconium	0(+)	0(−)	−	− 4%
Niobium	0(+)	0	0	+ 1.5%
Molybdenum	0(+)	−	−	− 4.5%
Rhodium	0(+)	+	+	+ 2%
Palladium	+	+	+	+ 3%
Silver	+	+	+	+ 4%
Cadmium	+	+(0)	+(0)	+ 4%
Indium	0(+)	+(0)	+	+ 2%
Tin	+(0)	+	+	+ 4%
Antimony	0(−)	0(−)	0(+,−)	− 1.5%

[a]   + : Data mostly above model curve.
      − : Data mostly below model curve.
     +,− : Data scattered noticeably relative to model curve with no dominant trend.
      0 : Data agree well with model curve.
    (...): Alternative possibility when trend is ambiguous.

[b]Indicate approximate maximum discrepancy observed between data and model
curve over 1-4 MeV range. Fluctuations may affect comparisons of data
and model results for the lighter elements. Percent values estimated to
nearest 0.5%. Positive sign implies data above model result.

TABLE 5. Percent Differences Between Optical-Model Parameters[a]

Element	$P_1 = V_o$ (1.9%)[b]			$P_2 = r_V$ (1.1%)[b]		
	Elemental[c]	Set A	Set B	Elemental[c]	Set A	Set B
Yttrium	+0.9	+0.3	+0.1	+0.4	+0.1	~ 0
Zirconium	+1.5	+0.2	+0.1	-0.6	+0.1	~ 0
Niobium	+1.7	+0.4	+0.1	~ 0	+0.1	~ 0
Molybdenum	+2.3*	+0.2	+0.1	-2.1*	+0.1	~ 0
Rhodium	-3.7*	+0.2	+0.1	+2.1*	+0.1	~ 0
Palladium	-2.4*	~ 0	+0.1	+1.3*	+0.1	~ 0
Silver	-0.8	+0.1	+0.1	+0.2	+0.1	~ 0
Cadmium	+1.2	-0.2	~ 0	-0.3	+0.1	~ 0
Indium	-2.0*	-0.2	~ 0	+1.1	+0.1	~ 0
Tin	+1.0	-0.4	~ 0	-0.5	~ 0	~ 0
Antimony	+0.9	-0.5	~ 0	-1.3*	~ 0	~ 0

Element	$P_3 = a_V$ (4.5%)[b]			$P_4 = W$ (11.5%)[b]		
	Elemental[c]	Set A	Set B	Elemental[c]	Set A	Set B
Yttrium	-0.3	+1.1	+0.7	+13.6*	-4.4	+1.6
Zirconium	+2.8	+1.0	+0.6	+6.6	-5.1	+1.9
Niobium	-2.7	+0.9	+0.6	-14.9*	-4.4	+1.5
Molybdenum	+8.5*	+0.8	+0.6	-2.0	-1.8	+2.0
Rhodium	+1.8	+0.4	+0.4	+11.8*	+4.3	+2.4
Palladium	-3.1	+0.2	+0.4	+7.3	+4.9	+2.8
Silver	-7.3*	+0.1	+0.4	-9.0	+4.4	+2.5
Cadmium	-4.6*	-0.2	+0.3	-3.9	+0.8	+3.1
Indium	+4.3	-0.4	+0.2	+21.4*	-2.3	+3.1
Tin	-0.6	-0.7	+0.2	+11.6*	-5.7	+3.7
Antimony	+5.9*	-0.9	+0.1	+13.5*	-4.9	+4.0

TABLE 5. Percent Differences Between Optical-Model Parameters[a] (Contd.)

Element	$P_5 = r_W$ (3.4%)[b]			$P_6 = a_W$ (15.0%)[b]		
	Elemental[c]	Set A	Set B	Elemental[c]	Set A	Set B
Yttrium	+3.9*	+0.4	+0.4	−17.3*	+5.9	+5.9
Zirconium	+1.3	+0.4	+0.4	+4.5	+5.7	+5.6
Niobium	−2.8	+0.3	+0.4	+22.7*	+5.5	+5.5
Molybdenum	+2.3	+0.3	+0.3	+8.0	+5.3	+5.3
Rhodium	−0.2	+0.2	+0.3	−3.0	+4.8	+4.8
Palladium	−5.2*	+0.2	+0.2	+13.6	+4.5	+4.6
Silver	−1.4	+0.2	+0.2	+21.8*	+4.6	+4.5
Cadmium	−5.1*	+0.2	+0.2	+19.6*	+4.2	+4.3
Indium	+6.1*	+0.1	+0.1	−20.6*	+4.1	+4.2
Tin	+2.3	+0.1	+0.1	−11.5	+3.9	+4.0
Antimony	+1.2	~ 0	+0.1	+14.1	+3.8	+3.9

[a]Percent differences relative to Set C regional parameters.
[b]Parameter standard deviations from Table 3.
[c]Values marked "*" exceed parameter standard deviations.

TABLE 6. Comparison of Total Cross Sections Calculated Using Elemental and Regional OM Parameters[a].

Element	Set A		Set B		Set C	
	Trend[b]	Maximum % Difference[c]	Trend[b]	Maximum % Difference[c]	Trend[b]	Maximum % Difference[c]
Yttrium	+,−	±1	−	−2.1	−	−3.8
Zirconium	−	−1	−	−1.7	−	−3.1
Niobium	−	−1.7	−	−3.2	−	−3.9
Molybdenum	−	−3.6	−	−3.3	−	−5.1
Rhodium	+	+1.9	+	+1.7	−	−1.4
Palladium	+,−	−2.3	+,−	−1.9	−	−2.0
Silver	−	−0.5	−	−0.6	−	−3.4
Cadmium	+,−	+0.9	−	−0.5	−	−1.8
Indium	+,−	+2.0	+	+1.1	+,−	+1.7
Tin	+	+3.6	+	+3.9	+	+2.7
Antimony	−	−3.2	−	−2.8	−	−2.9

[a]Percent values are differences in the regional model predictions relative to the elemental model predictions.

[b] +: Regional values mostly above elemental values.
   −: Regional values mostly below elemental values.
 +,−: No clear trend. Regional values found more or less uniformly above and below the elemental values.

[c]Positive difference implies regional value exceeds elemental value and conversely for negative difference.

TABLE 7. Identification of Best- and Worst-Fit Model Representations of Experimental Total Cross Section Data.

Element	Best		Worst	
	Model[a]	Maximum % Difference[b]	Model[a]	Maximum % Difference[c]
Yttrium	(Set A)	+6	Set C	+8.5
Zirconium	(Set A)	-3	Set C	+3
Niobium	Elemental	+1.5	Set C	+5
Molybdenum	(Set A)	+3	Set C	+4
Rhodium	Set B	+2	Set C	+2.5
Palladium	(Set A)	+2.5	Set C	+4.5
Silver	Elemental	+4	Set C	+7.5
Cadmium	Set B	+3	Set C	+5.5
Indium	Set B	±1	(Set C)	+3
Tin	(Set C)	+2	(Set A)	-1.5
Antimony	Elemental	+1	Set A	+4

[a](...): Choice somewhat ambiguous.
[b]Indicates approximate maximum discrepancy observed between data and model curve over 1-4 MeV. Fluctuations may affect comparisons of data and model results for the lighter elements. Percent values estimated to nearest 0.5%. Positive sign implies data above model result.

TABLE 8. Calculated Total Cross Sections and Uncertainties[a]

Rhodium [A = 103, (N−Z)/A = 0.12621]

E_n (MeV)	σ_T (b)	Error in σ_T	Correlation Matrix 1	2	3	4
1	6.39342	2.3%	1	(symmetric)		
2	5.03306	2.1%	0.44	1		
3	4.22298	2.2%	0.48	0.95	1	
4	3.88226	2.2%	0.59	0.83	0.95	1

Technetium [A = 99, (N−Z)/A = 0.13131]

E_n (MeV)	σ_T (b)	Error in σ_T	Correlation Matrix 1	2	3	4
1	6.42534	1.8%	1	(symmetric)		
2	4.89190	2.1%	0.78	1		
3	4.10271	2.1%	0.60	0.92	1	
4	3.80349	2.7%	−0.34	−0.07	0.09	1

Ruthenium [A = 101.17, (N−Z)/A = 0.12977[b]]

E_n (MeV)	σ_T (b)	Error in σ_T	Correlation Matrix 1	2	3	4
1	6.40563	1.9%	1	(symmetric)		
2	4.96532	2.1%	0.75	1		
3	4.16370	2.2%	0.59	0.94	1	
4	3.84247	2.2%	0.44	0.79	0.94	1

[a]Calculations employ Set C regional model parameters.
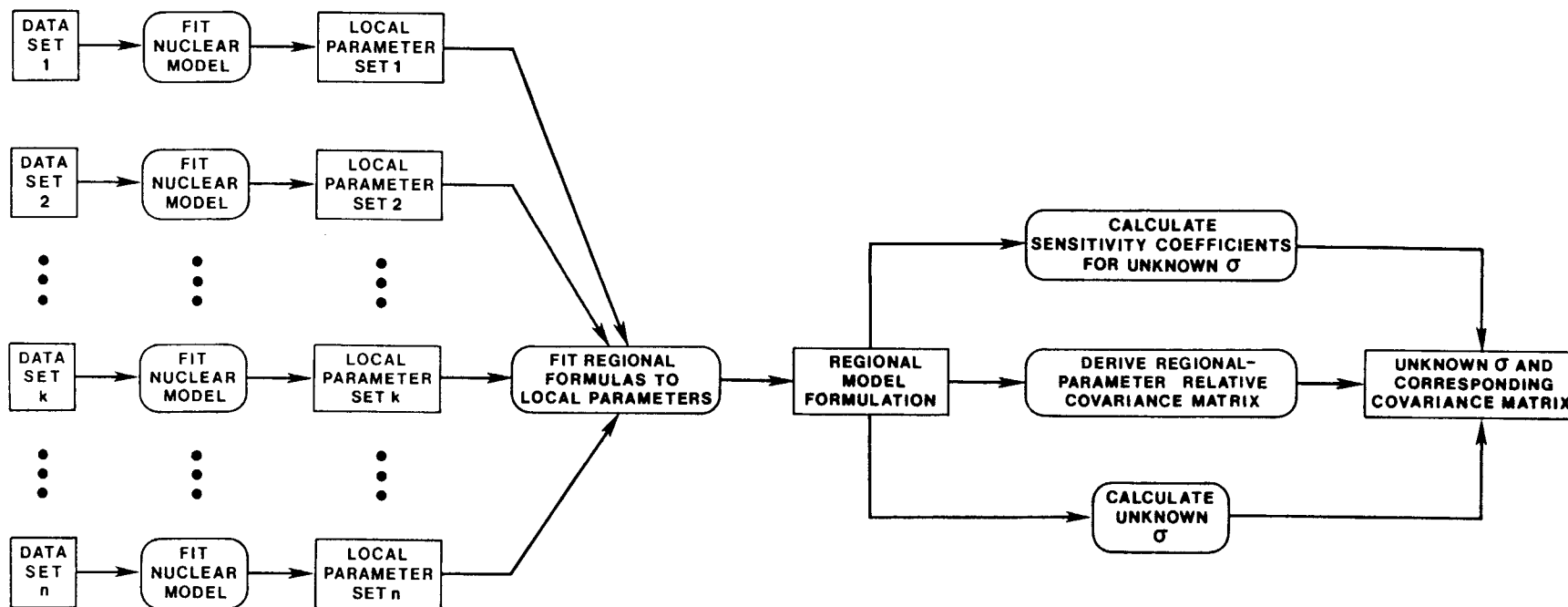[b]Elemental values derived as weighted average of isotopic values.

Fig. 1.   Logic diagram which outlines the basic aspects of the present
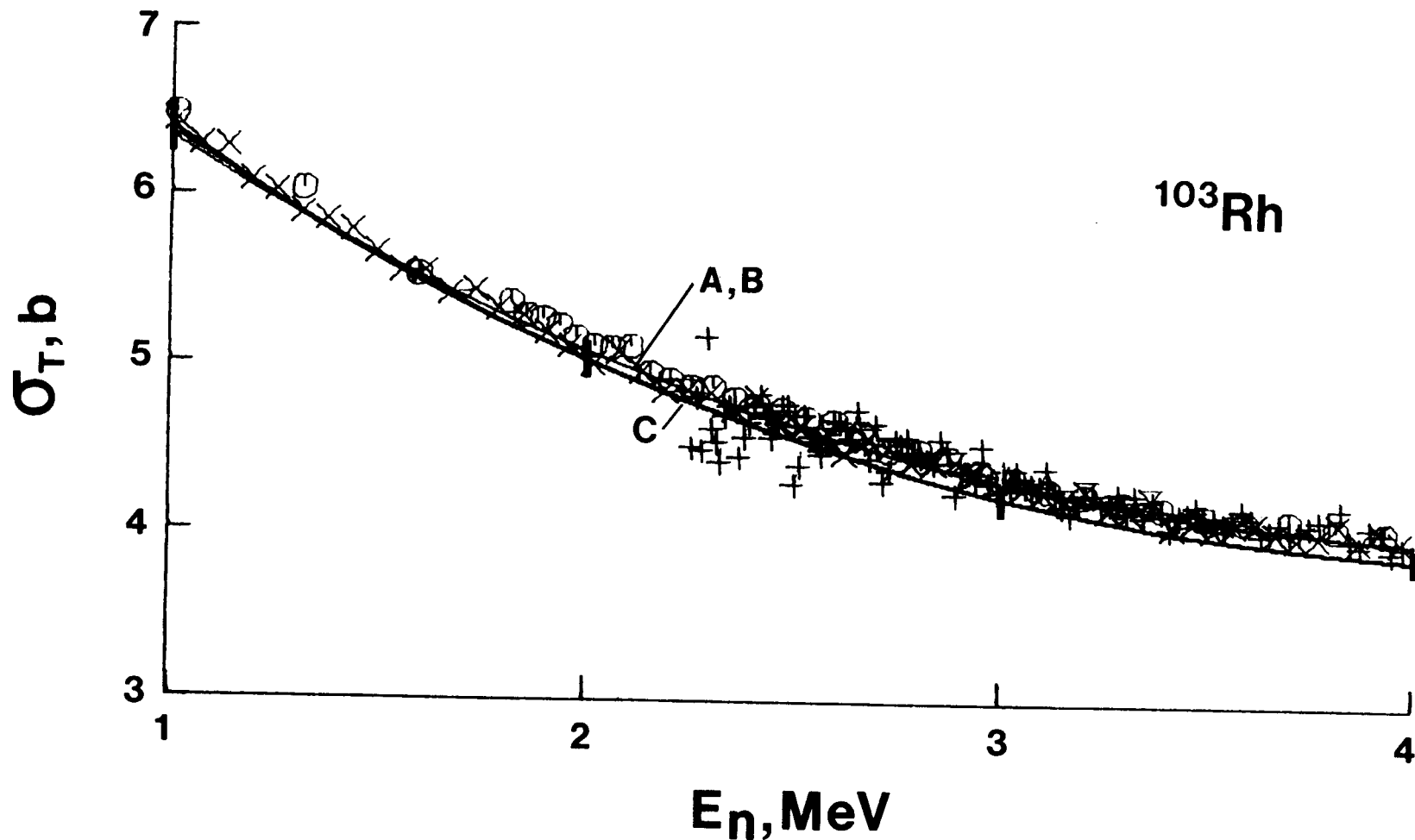method, as described in Section II of the text.

Fig. 2. Measured and calculated neutron total cross sections for ^{103}Rh. Curves A, B, and C are derived as discussed in Section III of the text. Curves A and B differ only slightly. The experimental data sets are: Ref. 25 (X), Ref. 35 (O), and Ref. 37 (+). The solid vertical bars centered on curve C at E_n = 1, 2, 3, and 4 MeV designate errors calculated using the present method.
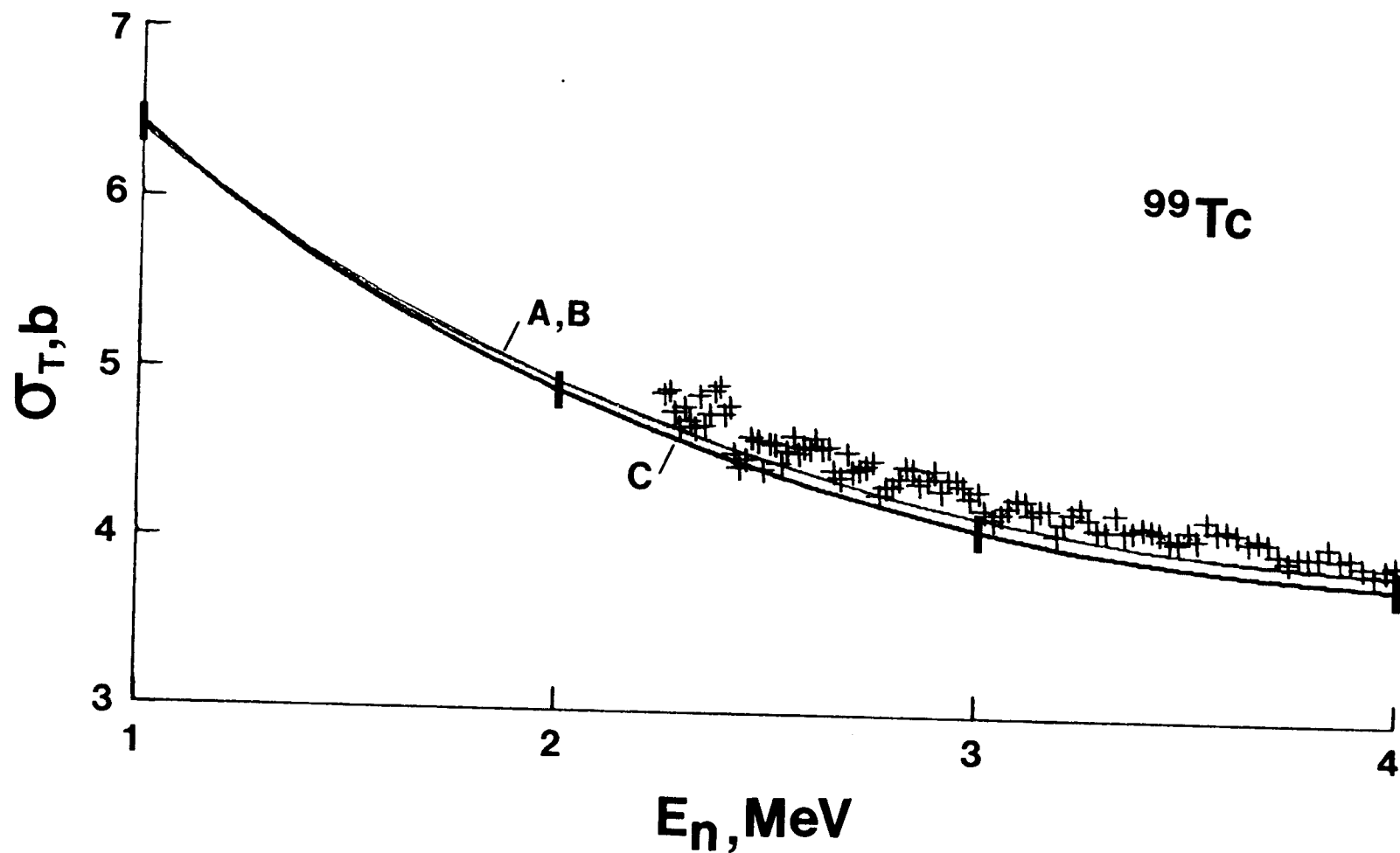
Fig. 3.   Measured and calculated neutron total cross sections for ^{99}Tc. Curves A, B, and C are derived as discussed in Section III of the text. Curves A and B differ only slightly. The experimental data set is from Ref. 37 (+). The solid vertical bars centered on Curve C at E_n = 1, 2, 3 and 4 MeV designate errors calculated using the present method.
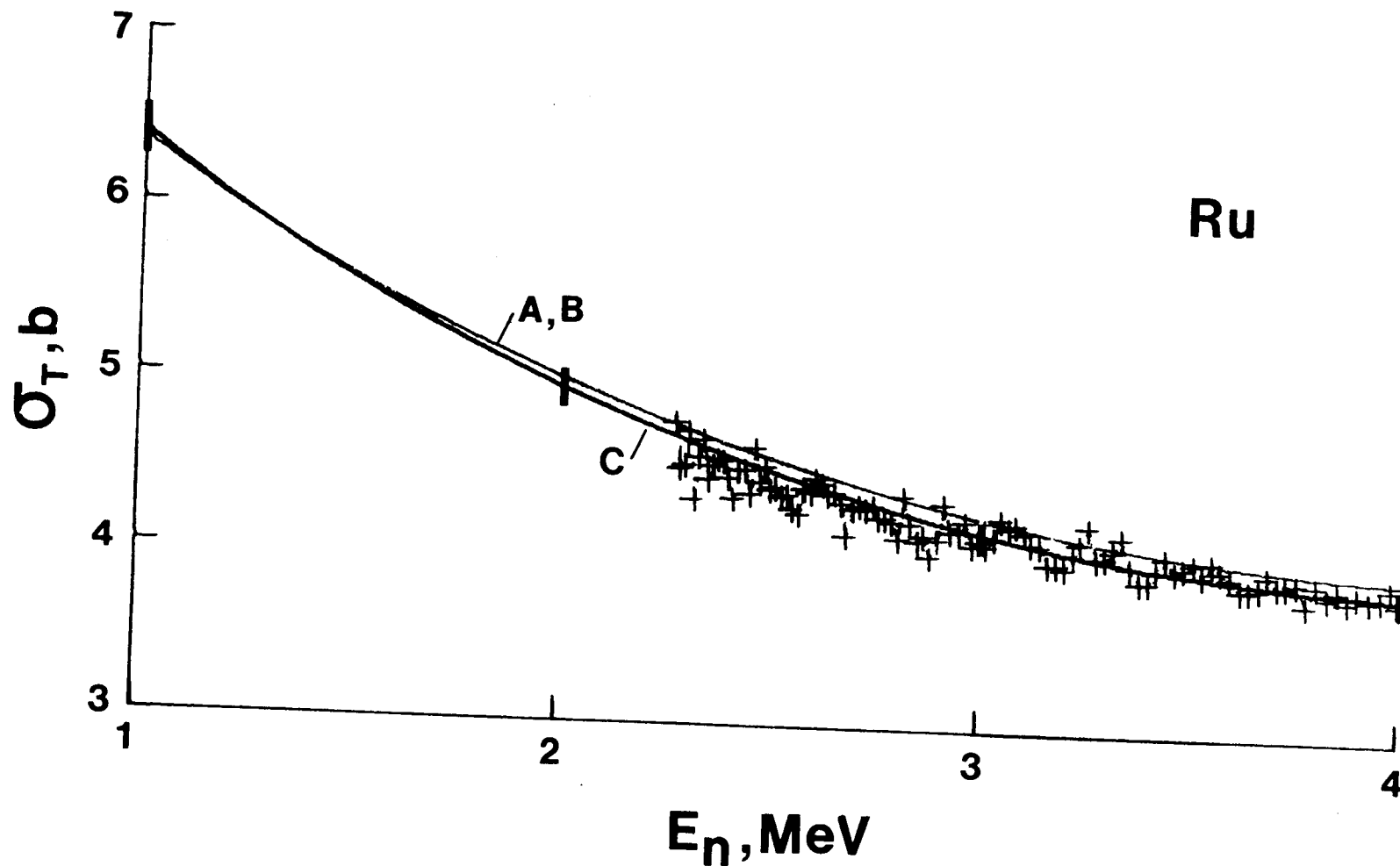
Fig. 4. Measured and calculated neutron total cross sections for elemental
Ru. Curves A, B, and C are derived as discussed in Section III of
the text. Curves A and B differ only slightly. The experimental
data set is from Ref. 37 (+). The solid vertical bars centered on
Curve C at E_n = 1, 2, 3 and 4 MeV designate errors calculated
using the present method.